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First-Order Phase Transition in the Quantum Adiabatic Algorithm

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We simulate the quantum adiabatic algorithm (QAA) for the exact cover problem for sizes up to $N = 256$ using quantum Monte Carlo simulations incorporating parallel tempering. At large N, we find that some instances have a discontinuous (first-order) quantum phase transition during the evolution of the QAA. This fraction increases with increasing N and may tend to 1 for $N \to \infty$.

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It is of great interest to know if an eventual quantum computer could solve a broad range of hard "optimization" problems more efficiently than a classical computer. An important class is the NP-hard category [1] (nondeterministic-polynomial-time-hard), for which it is believed that all classical algorithms take a time which grows exponentially with the problem size N.

The most promising approach to solving optimization problems on a quantum computer seems to be the quantum adiabatic algorithm (QAA), proposed by Farhi *et al.* [2]. The idea, which is related to quantum annealing [3], is that one adds to a "problem" Hamiltonian, $\mathcal{H}_P$, whose ground state represents a solution of a classical optimization problem, a noncommuting "driver" Hamiltonian, $\mathcal{H}_D$, so the total Hamiltonian is

$$\mathcal{H}(s) = (1 - s)\mathcal{H}_D + s\mathcal{H}_P, \tag{1}$$

where $s(t)$ is a *time-dependent* control parameter. $\mathcal{H}_P$ is expressed in terms of classical Ising spins taking values ± 1, or equivalently in terms of the z components of the Pauli matrices for each spin, $\hat{\sigma}_i^z$. The simplest driver Hamiltonian is then $\mathcal{H}_D = -\sum_{i=1}^{N} \hat{\sigma}_i^x$ where $\hat{\sigma}_i^x$ is the x-component Pauli matrix.

The control parameter $s(t)$ is 0 at $t = 0$, so $\mathcal{H} = \mathcal{H}_D$, which has a trivial ground state in which all 2^N basis states (in the $\hat{\sigma}^z$ basis) have equal amplitude. It then increases with t, reaching 1 at $t = \mathcal{T}$, where $\mathcal{T}$ is the runtime of the algorithm, at which point $\mathcal{H} = \mathcal{H}_P$. If the time evolution of $s(t)$ is sufficiently slow, the process will be adiabatic. Hence, starting the system in the ground state of $\mathcal{H}_D$, the system will end up in the ground state of $\mathcal{H}_P$ and the problem is solved. The time $\mathcal{T}$ required to find the ground state with significant probability is called the complexity. The bottleneck of the QAA is likely to be at one or more points where the energy gap from the ground state to the first excited state becomes very small, possibly due to a quantum phase transition.

Early numerical work [2,4] on very small systems, $N \leq 24$ (for a particular constraint satisfaction problem known as "exact cover 3," also called 1-in-3 sat), found that the complexity scaled polynomially with size, roughly as N^2, which caused a good deal of excitement. However, this power law complexity may be an artifact of the very small sizes studied, so it is of great interest to determine whether the complexity continues to be polynomial for much larger sizes or whether a "crossover" to exponential complexity is seen.

In previous work [5], we have used quantum Monte Carlo (QMC) simulations to investigate much larger sizes of the exact cover problem, up to $N = 128$. We found evidence that, while the median complexity is still polynomial, an increasing fraction of instances became very hard to equilibrate for the larger sizes. We have now considerably improved the algorithm, borrowing techniques from the spin glass field to speed up equilibration. We have therefore been able to understand much better these "troublesome" instances, and find that they have a first-order quantum phase transition. Furthermore, we have increased the range of sizes still further, up to $N = 256$, finding that the fraction instances with a first-order transition continues to increase with N, plausibly tending 1 for $N \to \infty$. The gap at a first-order phase transition is likely to be exponentially small [6,7], and hence lead to exponential complexity for the QAA.

We now describe the model and our results in more detail. To make a comparison with the earlier work, we study (essentially) the same model for $\mathcal{H}_P$ used by Farhi *et al.* [2]. This problem, known as exact cover, is a *random satisfiability* problem, a class which is known to be NP hard. In exact cover, there are N Ising spins and M "clauses" each of which involves three spins (chosen at

random). The energy of a clause is zero if one spin is -1 and the other two are 1, and otherwise the energy is a positive integer. The simplest Hamiltonian with this property is [8]

$$\mathcal{H}_P = \frac{1}{4}\sum_{\alpha=1}^{M}(\hat{\sigma}^z_{\alpha_1} + \hat{\sigma}^z_{\alpha_2} + \hat{\sigma}^z_{\alpha_3} - 1)^2, \tag{2}$$

where α_1, α_2, and α_3 are the three spins in clause α, and the $\{\hat{\sigma}^z_i\}(i = 1, \ldots, N)$ are Pauli matrices. In the absence of the driver Hamiltonian, the Pauli matrices can be replaced by classical Ising spins S_i taking values ± 1. An instance has a "satisfying assignment" if there is at least one choice for the spins where the total energy is zero. As the ratio $\alpha \equiv M/N$ is increased, there is a phase transition at α_s where the number of satisfying assignments goes to zero. The version used by Farhi *et al.* considers only instances with a *unique* satisfying assignment (USA), i.e., there is only *one* state with energy 0. This has the advantage that the gap $\Delta E(s)$ between the ground state and first excited state is greater than zero in both limiting cases, $\mathcal{H} = \mathcal{H}_D$ and $\mathcal{H} = \mathcal{H}_P$, but will have a *minimum* at an intermediate value $s = s^*$. In addition, it ensures that we work close to the satisfiability transition where the problem is particularly hard [9]. Hence here, and in the earlier work [5], we consider instances with a USA.

The method of generating instances with a USA is described in Ref. [5]. For each size N, we choose the number of clauses M which maximizes the probability of finding a USA, see Table I. The actual number of spins simulated N', is somewhat less than N due to isolated sites being omitted, and others that do not affect the complexity are also "pruned off" [5]. The value of $\alpha \equiv M/N$ seems to be close to the critical value $\alpha_s \simeq 0.626$ [10] for $N \to \infty$.

In QMC, we simulate an effective classical model with Ising spins $S_i(\tau) = \pm 1$ in which τ ($0 \le \tau < \beta \equiv T^{-1}$) is imaginary time. Following common practice, we discretize imaginary time into L_τ "time slices" each representing $\Delta\tau = \beta/L_\tau$ of imaginary time. We take $\Delta\tau = 1$.

As discussed previously [5], for $\beta\Delta E \gg 1$ (where $\Delta E \equiv E_1 - E_0$ is the energy gap), and $\tau \ll \beta$, the time-dependent correlation function

$$C(\tau) = \frac{1}{N'L_\tau}\sum_{i=1}^{N'}\sum_{\tau_0=1}^{L_\tau}\langle S_i(\tau_0 + \tau)S_i(\tau_0)\rangle, \tag{3}$$

is a sum of exponentials, i.e.,

$$C(\tau) = q + \sum_{n\ge 1} A_n \exp[-(E_n - E_0)\tau], \tag{4}$$

TABLE I. The sizes studied in the simulation.

N	16	32	64	128	192	256
M	12	23	44	86	126	166
α	0.7500	0.7188	0.6875	0.6719	0.6563	0.6484

where the A_n are constants and q, the spin glass order parameter, is given by

$$q = \frac{1}{N'}\sum_{i=1}^{N'}\langle S_i\rangle^2. \tag{5}$$

At large τ, the sum in Eq. (4) is dominated by the term corresponding to the first excited state ($n = 1$), and so $\Delta E \equiv E_1 - E_0$ can be obtained by fitting $\log[C(\tau) - q]$ against τ for large τ.

We have considerably improved the algorithm relative to that in Ref. [5] by incorporating "parallel tempering" [11,12], which has been very successful in speeding up simulations of spin glass systems. Whereas in spin glasses, one simulates copies of the system at different, close-by temperatures, in the quantum case, the copies are at different values of the control parameter s.

As already mentioned, the focus of the present study is to determine which instances have a first-order transition. Parallel tempering is very good at equilibrating the system on either side of the transition. However, it is still difficult (i) to determine exactly where the transition occurs, because both phases are metastable in the region where they are not the equilibrium state, and (ii) to accurately determine the minimum gap for first-order instances, because it is so small. We have performed runs starting the spins both from a random initial configuration and from the solution of the problem Hamiltonian. If we start by "seeding" the spins with the exact solution, we are confident that the Monte Carlo simulation is in the correct phase for s close to 1. It is also in the correct phase for small s because equilibration is easy in this region. Hence, if a long simulation starting the spins from the exact solution produces a sharp discontinuity, we feel that this is almost certainly the correct behavior.

In order to investigate whether or not a first-order transition occurs, we focus on the spin glass order parameter q defined in Eq. (5). The expectation value of q is always nonzero because of terms linear in the $\hat{\sigma}^z$ (magnetic field terms) in the Hamiltonian, Eq. (2). To determine the square of the average without bias, we simulated two copies of the spins at each value of s and evaluate $\langle S_i\rangle^2$ as $\langle S_i\rangle^{(1)}\langle S_i\rangle^{(2)}$. A representative result for an instance with a first-order transition is shown in Fig. 1. Note the very rapid increase in q over a very small range of s, and that the two curves on each side of the jump are obviously displaced vertically with respect to each other.

The dip before the jump clearly seen in Fig. 1 provides clear evidence for a two-phase coexistence, and hence a first-order transition, for the following reason. If both copies are in the same phase, then the mean value of $\langle S_i\rangle$ is the same in both copies. However, right at the first-order transition, one copy can be in one phase (the low-q phase, say) and the other copy in the other (high-q) phase. The average value of $\langle S_i\rangle$ can have different signs in the two phases for *some* sites i. Hence, the typical Hamming distance between the spin configurations in the two copies

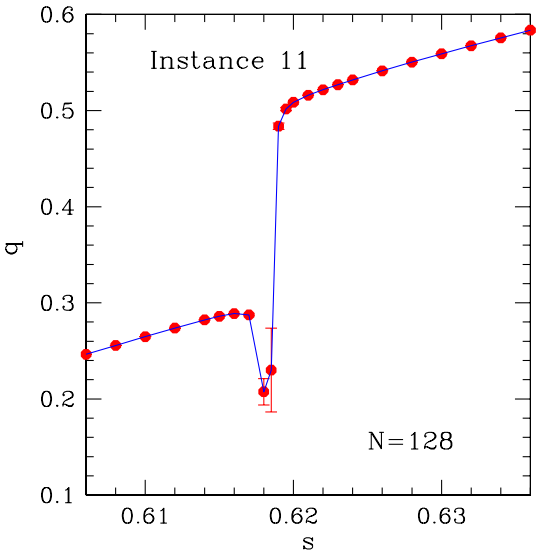

FIG. 1 (color online). An instance with a first-order transition with $N = 128$. Note the expanded horizontal scale.

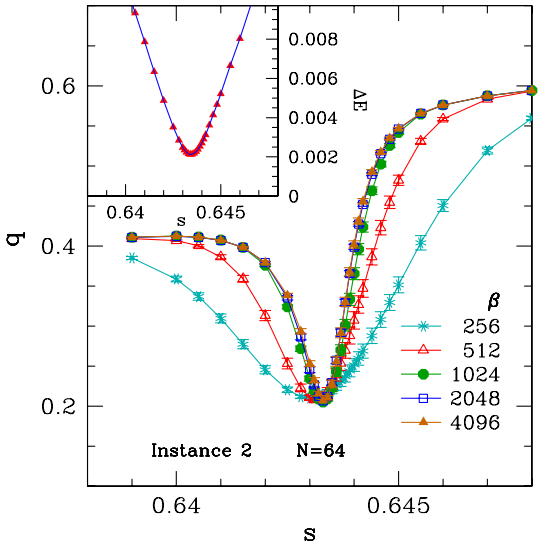

FIG. 2 (color online). The main figure shows the spin glass order parameter q, defined in Eq. (5), as a function of s for an instance with $N = 64$ which has a first-order transition. The different curves are for different values of β. The inset shows the energy gap ΔE as a function of s for $\beta = 2048$, indicating that $\Delta E_{\min} = 0.0021$ (same value was found for $\beta = 1024$ and 4096). From the main figure, one sees that the width of the finite-size rounding increases with $T \equiv 1/\beta$ for $T \gg \Delta E$ but is independent of T in the opposite limit $T \ll \Delta E$, as expected from Eq. (6). Note the expanded horizontal scale.

can be even greater (and so q even smaller) than when both copies are in the low-q phase. In every instance where we observed a sharp jump, this was proceeded by a dip. Hence, we use the dip as a precise criterion for a first-order transition.

Of course, even a first-order transition is rounded out for a finite-size system. To estimate the size of the rounding, we need to consider the two cases $\Delta E_{\min} \gg T$ and $\Delta E_{\min} \ll T$ separately, where $\Delta E_{\min}$ is the minimum value of the gap at the transition. If $\Delta E_{\min} \gg T$, δs is the range of s over which ΔE changes by an amount $\Delta E_{\min}$, whereas if $\Delta E_{\min} \ll T$, δs is the range of s over which ΔE changes by an amount equal to T. Hence,

$$\delta s = \begin{cases} \Delta E_{\min} (\frac{\partial \Delta E}{\partial s})^{-1}, & (\Delta E_{\min} \gg T), \\ T (\frac{\partial \Delta E}{\partial s})^{-1}, & (\Delta E_{\min} \ll T). \end{cases} \quad (6)$$

Figure 2 shows the finite-size rounding for an instance with $N = 64$, small enough that we can equilibrate through the (first-order) transition. For $\beta \lesssim 1024$, the width of the transition region increases as $\beta \equiv 1/T$ decreases, but for $\beta \gtrsim 1024$ the width is independent of β. For this instance, we find $\Delta E_{\min} = 0.0021$ as shown in the inset, so the width of the rounding becomes independent of T when $T \ll \Delta E$ as expected.

In Fig. 3, we plot the fraction of instances with a first-order transition. For each size, we have studied $N_{\text{inst}} = 50$ instances. If we denote the first-order fraction by r, then the error bar in r is $\sqrt{r(1-r)/(N_{\text{inst}}-1)}$. The figure shows that r increases rapidly with N and, very plausibly, tends to 1 for $N \to \infty$. We see that the first-order fraction is slightly greater than a half for $N = 128$. In our earlier work [5], we found that the *median* complexity continued to be polynomial up to $N = 128$ (the largest size studied). However, there is no contrast with the present work because, as already noted in Ref. [8], the models used are slightly different, and as a result, the crossover to a first-order transition occurs at a slightly lower value of N in the present model. The crossover to first order would have been seen in the earlier model if somewhat larger sizes had been studied.

Exponentially small gaps have been discussed before in the context of the QAA. Some time ago, one of us [13]

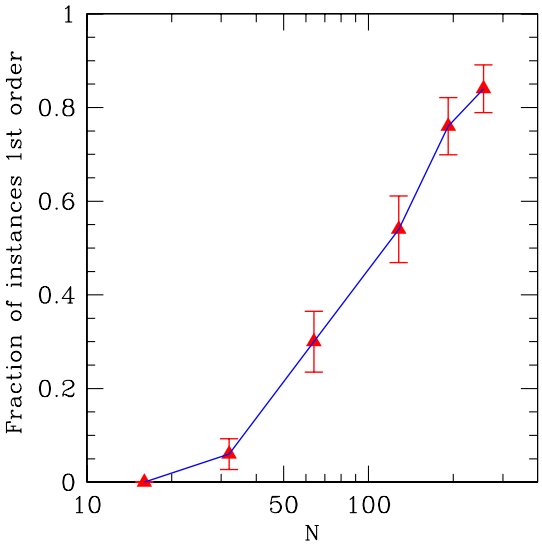

FIG. 3 (color online). The fraction of instances with a first-order transition (defined in the way discussed in the text) as a function of size. For each size, 50 instances were studied.

pointed out for a different problem, number partitioning, that the minimum gap is exponentially small, because of a transition between the states that are ''localized'' and ''extended'' in the computational basis.

Altshuler *et al.* [6] predict an exponentially small gap at large N for exact cover. Performing perturbation theory away from $s = 1$, they argue that there will be a level crossing between two ''localized'' states for s close to 1, at which point the ground state configuration changes abruptly. In our numerics, there is a big variation in the location of the first-order transition for a given size, but we do not detect a systematic shift towards $s = 1$ as the size increases. However, Altshuler *et al.* predict that $1 - s \sim N^{-1/8}$, which is probably too slow to be visible in our data. It will be interesting to investigate in future work whether the first-order transition found here is due to the mechanism they propose.

Farhi *et al.* [14] used a continuous imaginary time QMC method to study a very similar problem to ours, except that two solutions far away in Hamming space are ''planted'' into the Hamiltonian. This ensures that there is a finite probability of a first-order transition where the equilibrium state changes from one planted solution to another. By contrast, our work does nothing explicit to impose a first-order transition.

Jörg *et al.* [15] studied quantum annealing for the quantum random energy model (REM), the classical version of which [16] has a ''1-step replica symmetry breaking'' (also called a ''random first-order'') transition. Following Goldschmidt [17], they find a discontinuous quantum transition and argue that this leads to an exponentially small gap. They also observed that an exponentially small gap is seen in quantum versions of several models with random first-order transitions and suggested that this may be the general feature of all such models, including satisfiability [10,18]. However, the classical REM has zero spin glass order parameter q in the disordered phase [16] whereas classical random satisfiability models have lower symmetry because q is *always* nonzero due to the terms linear in $\hat{\sigma}^z$ in Eq. (2). Consequently, it is not obvious to us that the first-order quantum transition observed here is due to the same mechanism as that found [15] for the quantum REM. Very recently, a first-order transition has also been found in another model by Jörg *et al.* [19].

To conclude, we have a found a crossover to a first-order quantum phase transition during the evolution of the QAA for instances of exact cover with a unique satisfying assignment when the size becomes greater than about 100. It is possible that the complexity for *random* instances of exact cover could be different. We are therefore studying instances of exact cover with the USA constraint removed, and will also study other models in addition to exact cover.

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